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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Adjoint inverse modeling of a CO emission inventory at the city scale: Santiago de Chile's case" *by* P. Saide et al.

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Answers and comments to referee N1

We appreciate your review. Your comments refer to the ability of the model to reproduce observations, and the plausibility of applying inverse modeling techniques. We address one by one your comments, grouping them when suitable (in Italics).

Overall, we insist in the robustness of our results, and the suitability of the assumptions and modeling choices made.

In this study, the direct simulations showed (both for meteorology and surface concen-

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trations) that the model is not able to really reproduce the measurements. In this case, the inverse modeling process is not suitable: the differences between modeled and measured concentrations are so important that it is not realistic to report all possible error on CO surface emissions fluxes.

The Figure 3 shows not really good comparisons results between measured and modeled CO surface concentrations. The sentence, line 3, p.6333, 'we evaluate the model performance as adequate for the air quality simulations we are interested in, in particular during daytime' do not reflect what the curves show.

We disagree. We have made a rigorous comparison between model outputs and available observations (Only part of it shown in the paper due to space restrictions). Despite the complexity of the terrain, we find error statistics that are typical for state-of-the-art meso-scale meteorological models (e.g., Emery, 2001), and for air-quality models (e.g., Borrego et al, 2008).

Our inversion exercise excludes the periods of time when we are aware of severe disagreements between model outputs and observations (e.g., nighttime). Moreover, we discuss in detail whether our conclusions regarding the emission fluxes might be weakened by model errors other than emissions, finding our results to be robust. Also, previous studies using different models and periods of time, have shown similar biases attributable to systematic errors in emission fluxes (e.g., Gallardo et al, 2000; Schmitz, 2005).

Applying inverse methods to retrieve model parameters does not require of a "perfect" model neither are there any standards for defining "adequate" model errors for inverse modeling. An inverse method makes the model assumptions more explicit as well as the model and observation errors. An inverse method provides the best estimate of the sought parameters given a set of observations, model outputs and first guess, including its errors. Moreover, as stated earlier, when attributing discrepancies between model outputs and observations to emissions, we have been careful in discussing the plausibility of the hypothesis.

Overall, the model performance is comparable to that of other models of similar characteritics, and we find it appropriate to perform an inversion exercise. In addition, both the inversion procedure and its results are subject to a critical analysis, which makes us confident in the robustness of our results.

Even if a validation was done for another period, the better results are certainly due to the fact that the same kind of errors are corrected for both period: but probably not only emissions fluxes.

The methodology corrects the emission fluxes for the period for which the optimization is performed. The improvement found for the alternative period does not prove that the suggested fluxes are correct, it just corroborates our findings via the inverse method, supporting the robustness of our results. On the other hand, if other major model errors were at play, we would probably find no better results for the alternative period when applying the optimized inventory.

For the inverse modelling of CO, the appropriate estimation of BLH is a key point: the differences between model and observations may be only due to this representation of the atmosphere mixing state.

We share your opinion about how important it is to asses the error in vertical mixing. However, given that all stations are urban, an error in vertical mixing should result in a rather homogeneous bias in concentrations at all stations. However biases have a spatial distribution that cannot be explained solely by an error in vertical mixing. In other words, errors in vertical mixing cannot completely explain the differences between model and observations.

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The meteorological fields could be improved before retrying an inverse modeling experiment: if not, we can not be confident in the optimized emissions fluxes. In addition, a lot of model choices are done and debatable (not deposition, short spin-up etc.), leading to increased uncertainties in the results.

The authors say CO is a "long turn-over time of 2-4 months" species. Is it realistic to model the complete Santiago area with only a 24h spin-up model time? In addition, the authors say they started the run with null-values? Why? Is it possible to have a correct modelling of the pollution episode with this model set-up? without any realistic initial conditions? The results could be really improved by initializing the model with the available measurements, interpolated over the model domain (using kriging for example).

Even if dry deposition and scavenging are not dominant sources, it seems strange to not calculate these sinks for the CO behavior during the studied period. To prove that this choice is correct, it is necessary to present time series of precipitation and deposited fluxes of CO. The relative amount due to this sink must be discussed and compared to the global model error.

Regarding the model set-up, we made choices based upon previous work (our own and others), and numerous tests not necessarily reported in this paper due to space restrictions.

The choices made for the meteorological model (MM5) are largely based upon the multi-year experience of our colleagues at the Chilean Weather Office who provide an operational weather forecast for Central Chile at 4 km horizontal resolution, and that of other colleagues. In fact, we started with their custom set-up and changed it to account for the higher vertical and horizontal resolution we decided to use in order to get an improved representation of surface winds and vertical mixing. Unfortunately, since no vertical profiles are available for Santiago, our choices remain to some extent arbitrary. However, we tested several combinations, finding this to be the optimal one

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given the data available. In Table 1 we show as an example statistics for wind speed compared to benchmarks established in Emery (2001) and used in Gilliam et al (2006) showing that values fall within the guidelines.

Regarding the spin-up time for the dispersion simulations, we deemed a 24h spin-up time enough because in summer the Santiago basin gets "clean" from one day to another since there is almost no accumulation or recycling of pollutants. In Fig. 1 two simulations were performed. One starting on the 15th of January (no spin up) and the other starting the 2nd of January (14 days of spin up), both with initial conditions equal zero and the same configuration as in the Manuscript. Then it can be seen that initially both simulations differ, but after the first night, there is almost no difference in the peak in the morning, and the following concentrations remain the same. This shows that a 24h spin-up or even less is suitable when considering null initial conditions in the case of study.

The referee finds debatable that no deposition or scavenging is considered. As mentioned in the Manuscript, summers in Santiago are dry, so there is no scavenging. Sensitivity runs were made considering dry deposition showing almost no difference with a run without it (Fig. 2). Besides the very low deposition velocity of CO, the sources are very near to the observations leaving no time for deposition to occur.

The main purpose of this paper is to improve CO inverse modeling at the urban scale. The author stated than, decreasing the horizontal scale, the colocalisation of surface measurements becomes a problem. This effect depends on the resolution but also the meteorological conditions (dispersion effects) and the species reactivity. In the case of CO in Santiago, is it possible to quantify the relative weight of this co-localisation effect compared to all other model uncertainties? This has to be due to prove that the goal of the paper is not a second order problem compared to the emissions inventory uncertainty.

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In order to show that the co-localization problem is not a second order problem, Fig 3 shows the results from a synthetic run by only changing the factor applied. It can be seen that when no factor is applied, the tendency is to change only the emissions that are co-located with the observations due to the higher sensitivity obtained in these spots, obtaining retrieved emissions far from the real ones. When using real observations with no factor the results show a similar behavior. Adding regularization and its effects in inverse modeling is discussed in section 4.1.4.

The figure 2 shows comparisons between measured and modelled temperature. The vertical shape of the profiles tends to show a difference of inversions altitudes. This may induce large discrepancies on the boundary layer estimation (using the Louis formulation). It could be useful to see vertical profiles of temperature and wind, Richardson number for selected times (such as 07:00, 10:00, 13:00, 17:00, 20:00, 23:00) and the diagnosed boundary layer height (BLH).

The comparisons shown in Figure 2 in the paper illustrate that the model captures the regional patterns, synoptic changes and some of the relevant characteristics in the lower troposphere. It is not aimed at claiming a good representation of the boundary layer of the Santiago basin. The vertical profiles available are from Santo Domingo station that is by the coast some 100 km southwest from Santiago. Only two profiles per day are reported (12 and 00 UTC)

As stated earlier, vertical mixing is a key-issue. We would be glad to perform multiple sensitivity studies. However, vertical profiles are not available for Santiago for this period of time. We are happy that in the upcoming year a LIDAR will probably become available allowing a better assessment of boundary layer characteristics in Santiago.

The authors said that the model failed to represent very stable noctrunal conditions.

This is not a surprise and certainly a major problem of all existing regional models. But this could have a non negligible impact on inverse modeling results: are the authors able to quantify the impact of this kind of error several hours before the peak time of CO? An error made during the night will affect the transport and thus considerably change the modelled concentrations when they are compared to measurements.

Even though modeling errors could be produced during night hours, the amount of emissions during the night is very small (Fig 1 in the Manuscript) compared with the emissions in the peak hour. Then the peak in the morning is mainly explained by these emissions, and not to nocturnal ones. Figure 4 shows the results from a normal simulation and other where nocturnal emissions are set to zero showing the differences in the peak of the morning. Then, an error on the morning maximum is more likely to be explained by errors in morning emissions than errors in nocturnal emissions. Also, when looking at the observations, there is a mixed behavior in representing nocturnal concentrations (over and underestimation). That is why we think that in average the real effect on the peak in the morning due to nocturnal emissions and accumulation should not differ greatly from what the model shows, which is low as it has been said before.

In addition to nighttime modeling problems, the authors explain the model is not able to give correct results during the week-end. This is certainly due to a major change in the traffic fluxes (often observed in megacities). Is the inventory taken into account the week-end effect? If not, a first step would be to improve a little the inventory following this direction. To remove the week-end part of the modelled and measured concentrations for the inverse modeling is not correct: this is not possible to model a complete period and to inverse only the periods when the model gives realistic results. The inverse modeling process must be continuous in time to taken into account the transport and possible recirculations.

The available emission inventory is for a typical working day. For this work we choose to use the available information as such, and not to modify or compute other emissions before the inversion. This is why we do not introduce an emission inventory for the weekends. Since it is an error to consider the available emission inventory for weekends, these observations are not used for the inversion. Again, since the concentration from one day has almost no effect in the concentration for the following day, this simplification appears adequate. Inverse modeling does not need to be used sequentially.

In section 4.2, the authors restrict their inversion to fluxes greater than 0.5 mug/m2/s. Does it mean that, depending on time, the number of model grid cells (when an inversion process is performed), is not constant in time? This assumption is linked to another one: the inventories errors at one place are not correlated to errors at another place. But, this is certainly not the case since the same methodology is applied to built emissions over the whole domain. How the authors justify to spatially split the inversion process like this?

In section 4.2 is stated that the threshold is 0.5 mug/m2/s in temporal mean. This means that the emissions were averaged in time, and from this a spatial selection was taken using this threshold. Then the number of grid used for the inversion is constant in time (241 as stated in p6340 line 22). A comment will be introduced in this part to make the selection process clearer. The assumption of no correlation between emissions is discussed in section 4.1.2. We decided not to assume any value of correlation due to lack of information. Besides, even if no correlation is assumed, changes in emissions are spatially (Fig 11 in the manuscript) and temporary (Fig 12 in the manuscript) smooth, meaning that a certain degree of correlation is found in the results.

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Table 1. Model performance statistics calculated for wind speed and benchmarks proposed by Emery (2001).

	BIAS (m/s)	MAE (m/s)	IOA
WS benchmark	+/- 0.5	< 2	> 0.6
WS results	-0.21	0.98	0.76

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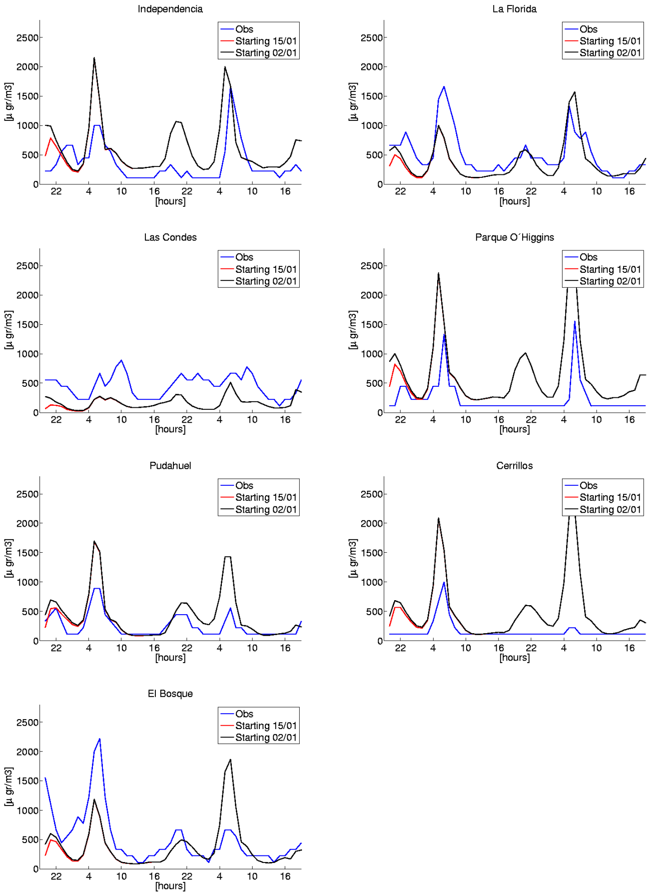

Fig. 1. Time series for 15th and 16th of January 2002 for observations and results of 2 runs of the dispersion model, one starting from the 15th and the other from 2nd, both with zero initial conditions.

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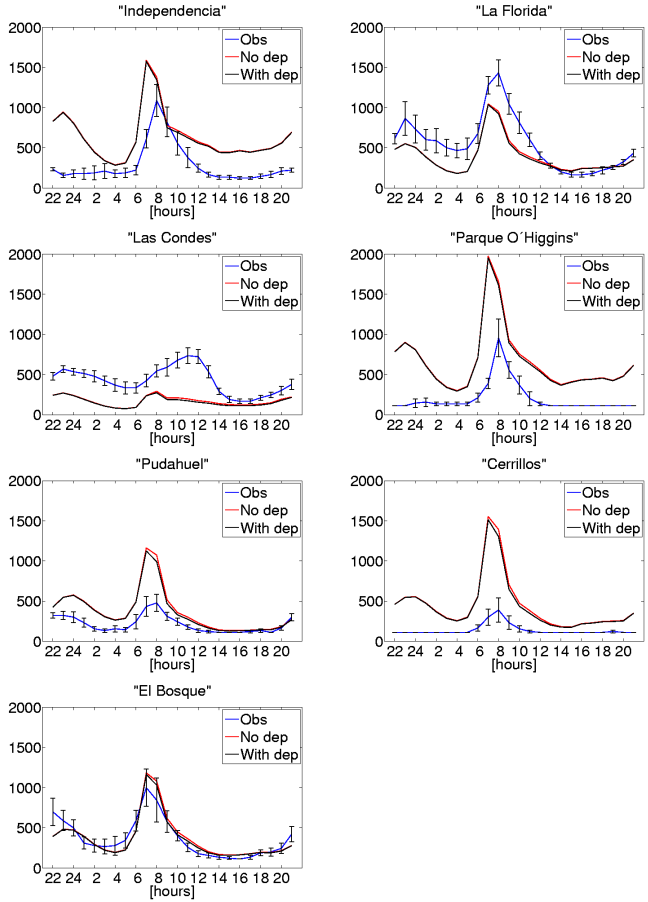

Fig. 2. Diurnal cycle for ten days of the inversion period for observations and results of 2 runs of the dispersion model: Using and not using deposition. Units in \unit{\mu}g/m3.

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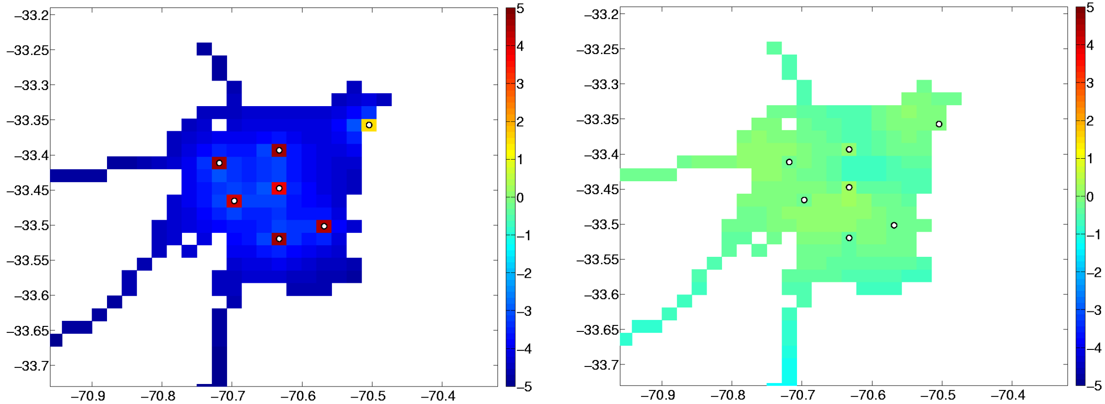

Fig. 3. ynthetic simulation results not using any factor on B matrix (left) and using the factor proposed in the manuscript (right). Mean in time of the difference between real and optimized EI.

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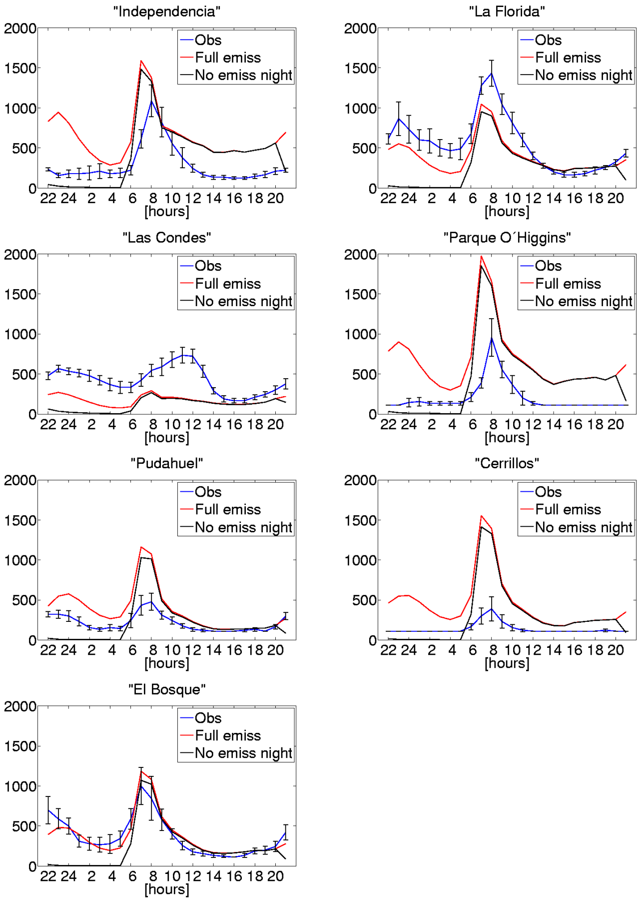

Fig. 4. Diurnal cycle for ten days of the inversion period for observations and results of 2 runs of the dispersion model: Using the complete emission inventory and setting emission to zero during the night.

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